New Classes of Nonseparable Space-Time Covariance Functions

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Outline

- Introduction
- Matérn Family of covariance functions
- Separable Modeling
- Nonseparable modeling
- Application and Numerical Studies
- Discussion
Notation, Stationarity

- A $p$-dimensional multivariate random field $\mathbf{Z}(\mathbf{x}) = \{Z_1(\mathbf{x}), \ldots, Z_p(\mathbf{x})\}^T$ defined on a spatial region $\mathcal{D} \subset \mathbb{R}^d$, $d \geq 1$

- A multivariate random field is second-order stationary (or just stationary) if the marginal and cross-covariance functions depend only on the separation vector $\mathbf{h} = \mathbf{x}_1 - \mathbf{x}_2$

$$C_{ij} : \mathbb{R}^d \to \mathbb{R}; C_{ij}(\mathbf{h}) := \text{cov}\{Z_i(\mathbf{x}_1), Z_j(\mathbf{x}_2)\}, \mathbf{h} \in \mathbb{R}^d$$

- Stationarity can be thought of as an invariance property under the translation of coordinates
A multivariate random field is isotropic if it is stationary and invariant under rotations and reflections,

\[ C_{ij} : \mathbb{R}_+ \cup \{0\} \rightarrow \mathbb{R}; \quad C_{ij}(||h||) := \text{cov}\{Z_i(x_1), Z_j(x_2)\}, \quad h \in \mathbb{R}^d \]

Isotropy or even stationarity are not always realistic, especially for large spatial regions, but sometimes are satisfactory working assumptions and serve as basic elements of more sophisticated anisotropic and nonstationary models.
Spatial Matérn

- **Matérn family**: correlation function (named after the Swedish forestry statistician Bertil Matérn)
  \[
  M(h|\nu, \alpha) := \frac{1}{2^{\nu-1}\Gamma(\nu)}(\alpha||h||)^\nu B_\nu(\alpha||h||), \quad h \in \mathbb{R}^d
  \]

  - \(B_\nu\), modified Bessel function of the second kind
  - \(\nu > 0\), smoothness and \(\alpha > 0\), scale parameters
  - for \(\nu = \text{odd integer}/2\) has a closed form expression
    - \(\nu = 1/2\), \(M(h|1/2, \alpha) = \exp(-\alpha||h||)\)
  - In the numerical analysis literature this kernel is also called the Sobolev kernel
Mean Square Differentiability here is defined as an $L^2$ limit

- e.g. an isotropic process is mean squared continuous if $E\{Z(s+h) - Z(s)\}^2 \to 0$, as $||h|| \to 0$
- $Z$ is $m$ times mean square differentiable if and only if $C^{(2m)}(0)$ exists and finite
- $Z$ is $m$ times mean squares differentiable if and only if $\nu > m$
Spatial Matérn

- Covariance functions for various levels of $\nu > 0$ (smoothness) and $\alpha > 0$ (scale) parameters
  - bigger $\nu$, the smoother $C$ around $0$
  - increasing as function of $\nu$,
    $M(h|\nu = 1/2, \alpha = 1) < M(h|\nu = 3/2, \alpha = 1)$
  - decreasing as function of $\alpha$,
    $M(h|\nu = 3/2, \alpha = 1) > M(h|\nu = 3/2, \alpha = 2)$

$$M(\nu = 1/2, \alpha = 1) = \exp(-||x||)$$
$$M(\nu = 3/2, \alpha = 2) = \exp(-2||x||)(1+2||x||)$$
$$M(\nu = 3/2, \alpha = 1) = \exp(-||x||)(1+||x||)$$
Univariate and Multivariate Matérn Family

- In the pure spatial setting: Matérn family (Matérn, 1960) has found widespread interest in recent years (Stein (1999), Guttorm and Gneiting (2006) for a historical account of this model)
- Multivariate Matérn: Marginal Spatial and cross-covariance as a function of Spatial lag are from Matérn (Gneiting et al. JASA (2011), Apanasovich et al. JASA (2012))
  - special case of multivariate space-time process was considered in Apanasovich et al. Biometrika (2010)
Positive Definiteness

The cross-covariance functions $C_{ij}(x_1 - x_2)$

\[ i, j = 1, p, x_1, x_2 \in D \]

must form $np \times np$ non-negative definite matrix for any positive integer $n$ and points $x_1, \ldots, x_n$ in $D$

\[ \{K(h)\}_{ij} = C_{ij}(h) \]

\[
\Sigma = \begin{pmatrix}
K(0) & K(x_1 - x_2) & \cdots & K(x_1 - x_n) \\
K(x_2 - x_1) & K(0) & \cdots & K(x_2 - x_n) \\
\vdots & \vdots & \ddots & \vdots \\
K(x_n - x_1) & K(x_n - x_2) & \cdots & K(0)
\end{pmatrix}
\]

\[ \text{var}(a^T Z) = a^T \Sigma a \geq 0, \forall a \in \mathbb{R}^{np}, \forall x_1, \ldots, x_n \in D, \forall n \in I \]
Positive Defitness

- Define the cross-spectral densities as \( f_{ij} : \mathbb{R}^d \rightarrow \mathbb{R} \) as

\[
f_{ij}(\omega) = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \exp(-i\mathbf{h}^T \omega) C_{ij}(\mathbf{h}) d\mathbf{h}, \quad \omega \in \mathbb{R}^d
\]

- \( i = \sqrt{-1} \)

- Cramer’s Theorem (slightly modified) A necessary and sufficient condition for \( K(\cdot) \) to be a valid (i.e., nonnegative definite), stationary matrix-valued covariance function is for the matrix function \( \{ f_{ij}(\omega) \}_{i,j=1}^p \) to be nonnegative definite for any \( \omega \) (Cramer 1940).
Separable Multivariate RF

- Separable forms: Mardia and Goodall (1993).

\[ K_{ij}(\mathbf{x}_1 - \mathbf{x}_2) = \sigma_{ij} K(\mathbf{x}_1 - \mathbf{x}_2), \quad i, j = 1, \ldots, p \]

- \( \Sigma = \{\sigma_{ij}\} \) is a positive definite matrix
- \( K(\cdot) \) is a valid correlation function
- **Problem**: same form of correlation for all \( i \)s and cross-correlations for all \( \{i, j\} \)s
  - E.g. \( K_{ij}(\mathbf{x}_1 - \mathbf{x}_2) = \sigma_{ij} \exp(-\alpha ||\mathbf{x}_1 - \mathbf{x}_2||) \) (same \( \alpha \))
Nonseparable Multivariate RF

- It is a challenging task
  - Fit marginal covariances, different $\alpha_{ii}, i = 1, \cdots, p$
    \[
    K_{ii}(x_1, x_2) := \exp(-\alpha_{ii} ||x_1 - x_2||), \alpha_{ii} > 0
    \]
- Evidence for spatial cross-correlation
  - How about
    \[
    K_{ij}(x_1, x_2) := \exp(-\alpha_{ij} ||x_1 - x_2||), \alpha_{ij} > 0, (\alpha_{ij} = \alpha_{ji})
    \]
  - WRONG! will NOT be a valid cross covariance unless $\alpha_{ij} = \alpha$
    for any $i, j = 1, \cdots, p$ (back to separability).
- Solution $K_{ij}(x_1, x_2) := \gamma(\alpha_{ij}) \exp(-\alpha_{ij} ||x_1 - x_2||)$ for some
  carefully chosen $\gamma(\cdot)$

\[ Z(x) = Aw(x), \]

- components of \( w(x) \in \mathbb{R}^p \) are iid spatial processes,
- \( A \) is \( p \times p \) full rank such that
\[ K_{ij}(x_1 - x_2) = \sum_{k=1}^{p} \rho_k(x_1 - x_2) A_{ik} A_{jk} \]

- The LMC can additionally be built from a conditional perspective (Royle and Berliner 1999; Gelfand et al. 2004)

- \[ Z_j(x) = \sum_{i=1}^{j-1} \alpha_i Z_i(x) + \sigma_j w_j(x) \]

- Drawbacks (In My Humble Frequentist Opinion)
  - with a large number of processes, the number of parameters can quickly become large
  - smoothness of any component of the multivariate random field is restricted to that of the roughest underlying univariate process.
A variant of a result of Gaspari et al. (2006) and theorem 1 of Majumdar and Gelfand (2007)

Suppose that $c_1, \ldots, c_p$ are real-valued functions on $\mathbb{R}^d$ which are both integrable and square-integrable.

$$C_{ij}(h) = (c_i \ast c_j)(h), \quad \text{for } i, j = 1, \ldots, p$$

$\ast$ denotes the convolution operator

Drawbacks

- Although some closed-form expressions exist, this method usually requires Monte Carlo integration
- The models for which the closed form expressions exist are somewhat rigid
Covariance convolution: Matérn

Recall

\[ K_{ij}(h) = (c_i \ast c_j)(h), \quad \text{for } i, j = 1, \ldots, p \]

From Gneiting, Kleiber, Schlather (2012)

- \(c_i\) are being suitably normalized Matérn functions with common scale \(\alpha > 0\) and smoothness \(\nu_i/2 - d/4\)
- Hence, recall \(M(\cdot | \cdot)\) is a univariate Matérn

\[
K_{ij}(h) = \gamma(\nu_i, \nu_j)M\{h|\nu_i + \nu_j)/2, \alpha\}
\]

\[
\gamma(\nu_i, \nu_j) = \frac{\{\Gamma(\nu_i + d/2)\}^{1/2}}{\{\Gamma(\nu_i)\}^{1/2}} \frac{\{\Gamma(\nu_j + d/2)\}^{1/2}}{\{\Gamma(\nu_j)\}^{1/2}} \frac{\Gamma((\nu_i + \nu_j)/2)}{\Gamma((\nu_i + \nu_j + d)/2)}
\]
The key idea is to represent $i$-th vector’s component ($i = 1, \cdots, p$ for $p$ dimensional random field) as a point in a $k$-dimensional space ($1 \leq k \leq p$), $\xi_i = (\xi_{i1}, \cdots, \xi_{ik})^T$; and include it inside the covariance function

$$K_{ij}(x_1, x_2) = \tilde{K}\{(x_1, \xi_i), (x_2, \xi_j)\}$$

Similar to multidimensional scaling with latent measures of dissimilarities between vector’s components

The idea of using Latent Dimensions is very general

A special case that is discussed in the paper in relationship to Matérn is

\[ -\alpha_{ij}^2 \] form a conditionally nonnegative definite matrices

\[ K_{ij}(h) = \gamma(\alpha_{ij}) M\{h|\nu, 1/\alpha_{ij}\} \]

\[ \gamma(\alpha_{ij}) = 1/\alpha_{ij}^d \]
Mixture Representation

There a well-known closure properties for matrix-valued covariance functions (Reisert and Burkhardt 2001) to use for sufficient conditions for validity.

Suppose that for all \( r \in L \subset \mathbb{R}^l \), \( C_r : \mathbb{R}^d \to \mathbb{R} \) is a (univariate) correlation function, while \( D_r \in \mathbb{R}^{p \times p} \) is symmetric and nonnegative definite. Suppose furthermore that for all \( h \in \mathbb{R}^d \) the product \( D_r C_r(h) \) is componentwise integrable with respect to the positive measure \( F \) on \( L \). Then

\[
C(h) = \int_L D_r C_r(h) dF(r)
\]

Drawback: it is hard to come up with all the elements
Mixture Representation: Matérn

- From Gneiting, Kleiber, Schlather (2012): only for byvariate
Multivariate GRF and SPDE approach: Matérn

- By Hu, Simpson, Lindgren, Rue
- The advantage: there is no explicit dependency on the theory of positive definite matrix
- Next talk. Stay tuned!
Recall cross-spectral densities are

\[
f_{ij}(\omega) = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \exp(-\iota h^T \omega) C_{ij}(h) dh, \quad \omega \in \mathbb{R}^d
\]

\[\iota = \sqrt{-1}\]

Need to show that \(\{f_{ij}(\omega)\}_{i,j=1}^P\) is nonnegative definite for any \(\omega\)

From Apanasovich, Genton, Sun (2012) JASA ”A Valid Matérn Class of Cross-Covariance Functions for Multivariate Random Fields with any Number of Components”
Main Result

- **The flexible multivariate Matérn model**
  1. Marginal parameters: $\nu_{ii}$, $\alpha_{ii}$, $\sigma_{ii}$;
  2. Somewhat flexible cross-covariance parameters: $\sigma_{ij}$;
  3. Extra parameters $\nu_{ij} = \nu_{ji}$, $\alpha_{ij} = \alpha_{ji}$, $i \neq j$ with some constraints which involve nontrivial functions of $\nu_{ii}, \nu_{jj}, \alpha_{ii}, \alpha_{jj}$ and $\sigma_{ij}$

- **Recall:** Gneiting, Kleiber, Schlather (2012) for $p \geq 3$
  1. Marginal parameters: $\nu_{ii}$, $\alpha_{ii} = \alpha$, $\sigma_{ii}$;
  2. Less flexible cross-covariance parameters: $\sigma_{ij}$;
  3. Other parameters for cross-covariances $\nu_{ij} = (\nu_{ii} + \nu_{jj})/2$, $\alpha_{ij} = \alpha$, $i \neq j$
Main Result

- **Theorem** The flexible multivariate Matérn model provides a valid structure if there exists $\Delta_A \geq 0$, such that
  
  1. $\nu_{ij} - (\nu_{ii} + \nu_{jj})/2 = \Delta_A (1 - A_{ij})$, $i, j = 1, \cdots, p$, where $0 \leq A_{ij}$ form a valid correlation matrix;
  
  2. $-\alpha_{ij}^2$, $i, j = 1, \cdots, p$, form a conditional nonnegative definite matrix;
  
  3. $\sigma_{ij} \alpha_{ij}^{2\Delta_A + \nu_{ii} + \nu_{jj}} \frac{\Gamma(\nu_{ij} + d/2)}{\Gamma\{(\nu_{ii} + \nu_{jj})/2 + d/2\} \Gamma(\nu_{ij})}$, $i, j = 1, \cdots, p$, form a nonnegative definite matrix
Parameterization

- **marginal parameters:** $\alpha_{ii}$, $\nu_{ii}$, $\sigma_{ii}$
- **cross-covariance parameters**
  - $\nu_{ij} = (\nu_{ii} + \nu_{jj})/2 + \Delta_B(1 - R_{A,ij})$, $\Delta_A > 0$, $R_A$ is a valid correlation matrix with nonnegative entries $i, j = 1, \cdots, p$
  - $\alpha^2_{ij} = (\alpha^2_{ii} + \alpha^2_{jj})/2 + \Delta_B(1 - R_{B,ij})$, $\Delta_B > 0$, $R_B$ is a valid correlation matrix with nonnegative entries $i, j = 1, \cdots, p$
  - $\rho_{ij} = R_{V,ij}\gamma(\alpha_{ii}, \alpha_{jj}, \alpha_{ij}, \nu_{ii}, \nu_{jj}, \nu_{ij})$, $\gamma(\cdot)$ is a well defined function (see the paper), $R_V$ is a valid correlation matrix
- Hence to model cross-covariance parameters, one need to choose parameterization for correlation matrices
  - In case of a small number of variables, $p$, one can use equicorrelated $R_L$s, so that $R_{L,ij} = \rho_L$, $i \neq j$, $L \in \{A, B, V\}$
  - latent dimension $R_{L,ij} = \exp(-||\xi_{L,i} - \xi_{L,j}||)$, for vectors $\xi_{L,i} \in \mathbb{R}^k$, $1 \leq k \leq p$, under constraints discussed in Apanasovich and Genton (2010).
Special Case

- The least flexible parametrization

\[ \nu_{ij} = \frac{\nu_{ii} + \nu_{jj}}{2}, \quad \alpha_{ij} = \left( \frac{\alpha_{ii}^2 + \alpha_{jj}^2}{2} \right)^{1/2}, \quad \sigma_{ij} = (\sigma_{ii} \sigma_{jj})^{1/2} \rho_{ij} \]

\[ \rho_{ij} = \frac{\alpha_{ii}^{\nu_{ii}} \alpha_{jj}^{\nu_{jj}}}{\alpha_{ij}^{2\nu_{ij}}} \frac{\Gamma(\nu_{ij})}{\Gamma^{1/2}(\nu_{ii}) \Gamma^{1/2}(\nu_{jj})} R_{ij} \]

where \( R_{ij} \) is a valid correlation matrix

- Marginal parameters: \( \nu_{ii}, \alpha_{ii}, \sigma_{ii} \)
- No extra parameters to model \( \nu_{ij}, \alpha_{ij} \)
- Extra parameters involved in cross-covariances: \( R_{ij} \)
Simulations

- we conducted simulation studies for the cases $p = 2, 3$.
- The simulation scenarios are motivated by a meteorological dataset discussed by Gneiting et al. (2012). It consists of temperature and pressure observations, as well as forecasts, at 157 locations in the North American Pacific Northwest. In our simulation studies, we use these same 157 locations and generate a bivariate or trivariate spatial Gaussian random field with multivariate Matérn cross-covariance structure.
Table 1: Summary statistics of parameter estimation of the bivariate ($p = 2$) Matérn model over 1,000 replicates.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>True</th>
<th>Min</th>
<th>$Q_1$</th>
<th>Median</th>
<th>Mean</th>
<th>$Q_3$</th>
<th>Max</th>
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<tbody>
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<td>$\alpha_{11}$</td>
<td>0.02</td>
<td>0.0095</td>
<td>0.0193</td>
<td>0.0217</td>
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Table 2: Summary statistics of parameter estimation of the trivariate ($p = 3$) Matérn model over 1,000 replicates.
Simulations

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<tr>
<th>Parameter</th>
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<th>Min</th>
<th>$Q_1$</th>
<th>Median</th>
<th>Mean</th>
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</table>
Simulations
Wind speed/Temperature/Pressure

- Meteorological dataset: at 120 locations in Oklahoma
- 100 locations for model fitting; 20 locations to evaluate the wind speed prediction performance.
- Fit a random field after removing a quadratic trend of longitude, latitude and elevation
Results: Trivariate Spatial Field

- Estimates of parameters for our flexible trivariate Matérn model

<table>
<thead>
<tr>
<th>$\hat{\nu}_{11}$</th>
<th>$\hat{\nu}_{22}$</th>
<th>$\hat{\nu}_{33}$</th>
<th>$\hat{\nu}_{12}$</th>
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<td>1.05</td>
<td>1.37</td>
<td>1.64</td>
</tr>
<tr>
<td>$1/\hat{\alpha}_{11}$</td>
<td>$1/\hat{\alpha}_{22}$</td>
<td>$1/\hat{\alpha}_{33}$</td>
<td>$1/\hat{\alpha}_{12}$</td>
<td>$1/\hat{\alpha}_{13}$</td>
<td>$1/\hat{\alpha}_{23}$</td>
</tr>
<tr>
<td>14.5</td>
<td>20.0</td>
<td>11.0</td>
<td>15.6</td>
<td>11.9</td>
<td>13.0</td>
</tr>
</tbody>
</table>
Results: Trivariate Spatial Field

Marginal correlation and cross-correlation fits: solid curves = flexible, and dashed = parsimonious

Figure: Marginal correlation and cross-correlation fits for wind speed, temperature, and pressure: solid curves for the flexible trivariate Matérn model and dashed curves for the parsimonious trivariate Matérn model.
Results: Trivariate Spatial Field

<table>
<thead>
<tr>
<th>Model</th>
<th>#Para</th>
<th>Loglik</th>
</tr>
</thead>
<tbody>
<tr>
<td>5. Flexible Matérn ($\Delta_{A,ij}, \Delta_{B,ij}$)</td>
<td>+8</td>
<td>−34,359.6</td>
</tr>
<tr>
<td>4. $\nu_{ij} = (\nu_{ii} + \nu_{jj})/2 + \Delta_A, \alpha_{ij}^2 = (\alpha_{ii}^2 + \alpha_{jj}^2)/2 + \Delta_B$</td>
<td>+4</td>
<td>−35,125.6</td>
</tr>
<tr>
<td>3. $\nu_{ij} = (\nu_{ii} + \nu_{jj})/2 + \Delta_A, \alpha_{ij}^2 = (\alpha_{ii}^2 + \alpha_{jj}^2)/2$</td>
<td>+3</td>
<td>−35,615.9</td>
</tr>
<tr>
<td>2. $\nu_{ij} = (\nu_{ii} + \nu_{jj})/2, \alpha_{ij}^2 = (\alpha_{ii}^2 + \alpha_{jj}^2)/2 + \Delta_B$</td>
<td>+3</td>
<td>−36,193.3</td>
</tr>
<tr>
<td>1. Parsimonious: $\nu_{ij} = (\nu_{ii} + \nu_{jj})/2, \alpha_{ij} = \alpha$</td>
<td>0</td>
<td>−36,572.3</td>
</tr>
</tbody>
</table>
Cokriging Trivariate Spatial Field

- temperature and pressure at all 120 locations, wind speed at 100, predict the wind speed at 20
- Different predictive scores for wind speed

<table>
<thead>
<tr>
<th>Model</th>
<th>MSPE</th>
<th>MAE</th>
<th>LogS</th>
<th>CRPS</th>
</tr>
</thead>
<tbody>
<tr>
<td>Flexible</td>
<td>17.5</td>
<td>3.3</td>
<td>4.0</td>
<td>4.4</td>
</tr>
<tr>
<td>Parsimonious</td>
<td>24.8</td>
<td>3.8</td>
<td>4.4</td>
<td>5.3</td>
</tr>
</tbody>
</table>

- Prediction errors for the flexible (magenta) and parsimonious (blue) for each of the 20 left-out locations